Terephthalic acid, heptyl 2-nitro-3-methylbenzyl ester

Inchi: InChI=1S/C23H27NO6/c1-3-4-5-6-7-15-29-22(25)18-11-13-19(14-12-18)23(26)30-16-20-
InchiKey: NIBKLAKXUKDWNW-UHFFFAOYSA-N
Formula: C23H27NO6
SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OCc2cccc(C)c2[N+](=O)[O-])cc1
Mol. weight [g/mol]: 413.46

Physical Properties

Property code	Value	Unit	Source
gf	-93.58	kJ/mol	Joback Method
hf	-579.76	kJ/mol	Joback Method
hfus	59.18	kJ/mol	Joback Method
hvap	108.23	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	5.387		Crippen Method
mcvol	319.710	ml/mol	McGowan Method
pc	1366.68	kPa	Joback Method
rinpol	2864.00		NIST Webbook
rinpol	2864.00		NIST Webbook
tb	1098.36	K	Joback Method
tc	1347.31	K	Joback Method
tf	727.30	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.28	J/mol×K	1098.36	Joback Method
cpg	1059.82	J/mol×K	1139.85	Joback Method
cpg	1067.77	J/mol×K	1181.34	Joback Method
cpg	1074.20	J/mol×K	1222.84	Joback Method
cpg	1079.15	J/mol×K	1264.33	Joback Method
cpg	1082.69	J/mol×K	1305.82	Joback Method
cpg	1084.87	J/mol×K	1347.31	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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